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## Phase Transitions of Organic-Inorganic Hybrid Perovskites under Pressure

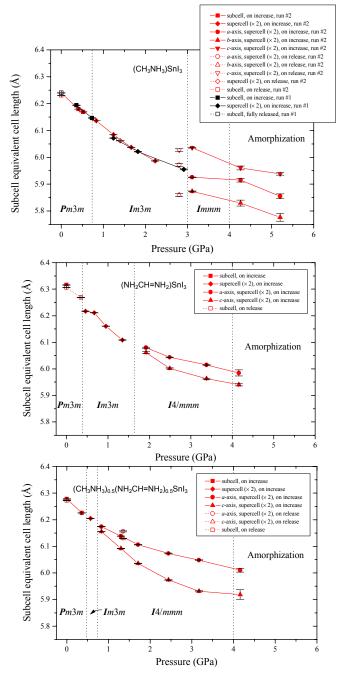
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Hybrid perovskites, based on a molecular-scale composite of inorganic and organic components, provide a substantial opportunity for tailoring combined functionality within a single material or new phenomenon that result from the interaction between the organic and inorganic subunits. These form a diverse structural group in which the effective dimensionality of the inorganic framework can be controlled from zero-dimension to layered oriented

systems. 1 The ordering and hydrogen bonding of the organic cations are known to change as a function of temperature and give rise to various structural phase transitions. Knowledge on pressure-induced changes in the organicinorganic interaction and its structure is, however, scarce, and we have initiated a systematic study to explore the high-pressure behaviors of various hybrid perovskites using monochromatic synchrotron X-ray and a diamond-anvil cell. Three samples in 3D hybrid perovskite systems, (CH<sub>3</sub>NH<sub>3</sub>)SnI<sub>3</sub>, (NH<sub>2</sub>CH=NH<sub>2</sub>)SnI<sub>3</sub>,  $(CH_3NH_3)_{0.5}(NH_2CH=NH_2)_{0.5}SnI_3$ , were chosen to investigate the effect of varying number of hydrogen-bonding site per A cation on its pressure response. As pressure increases above 0.5 GPa, all these materials show doubling of their cubic cell edges, mainly due to the tilting of the respective SnI<sub>3</sub> framework. The supercell structure of (CH<sub>3</sub>NH<sub>3</sub>)SnI<sub>3</sub> transforms to an orthorhombic phase above 3.0 GPa, probably as a result of increased ordering of the organic cation, whereas those of (NH<sub>2</sub>CH=NH<sub>2</sub>)SnI<sub>3</sub> and  $(CH_3NH_3)_{0.5}(NH_2CH=NH_2)_{0.5}SnI_3$  transform into tetragonal phases above 1.5 GPa and 1.0 GPa, respectively. In all cases, further increase in pressure above 4 GPa results in amorphization. which is reverted upon pressure release. This suggests the organic cations act as a template under high pressure and impart structural memory effect during amorphization of the inorganic frameworks.

Figure. Pressure dependence of the unit cell edge lengths of (CH $_3$ NH $_3$ )SnI $_3$  (upper), (NH $_2$ CH=NH $_2$ )SnI $_3$  (middle) and (CH $_3$ NH $_3$ ) $_{0.5}$ (NH $_2$ CH=NH $_2$ ) $_{0.5}$ SnI $_3$  (lower).

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## References:

[1] Mitzi, D. B. Synthesis, structure, and properties of organic-inorganic perovskites and related materials *In* Progress in inorganic chemistry Vol 48, Karlin, K. D. (Ed), John Wiley & Sons, 1999.